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High Performance Computing of Magnetic Fusion Plasma Physics Using Particle-in-Cell Technique

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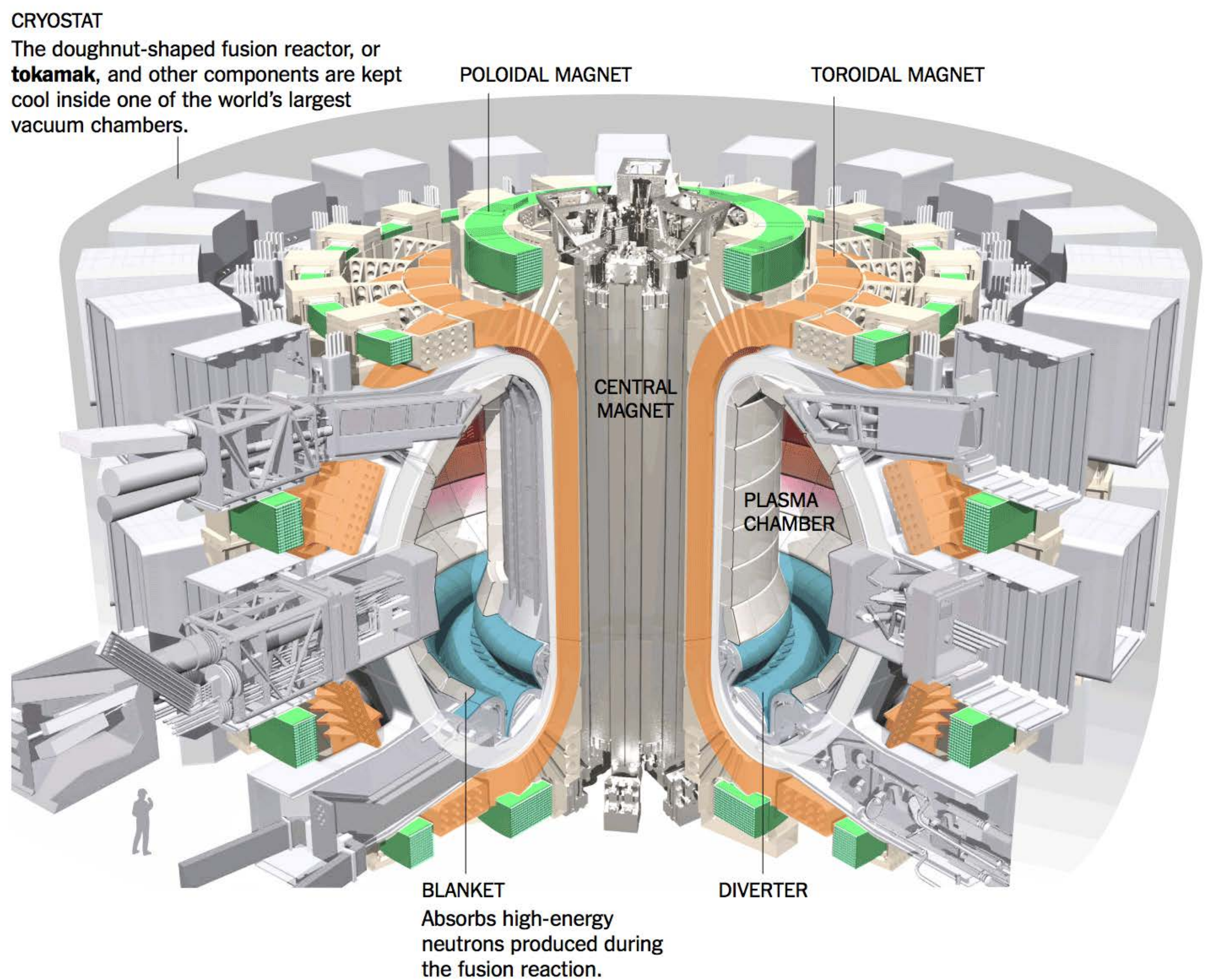
Outline

- Introduction to tokamak plasma physics
- 5D gyrokinetic equations and far-from-equilibrium edge physics in magnetic fusion
- Introduction to numerical PIC schemes that are used for magnetic fusion research
- Introduction to the extreme scale PIC code XGC for magnetic fusion plasma physics
- Significant example solutions that are only possible on leadership class HPCs

The New York Times *A Dream of Clean Energy at a Very High Price*

By HENRY FOUNTAIN MARCH 27, 2017

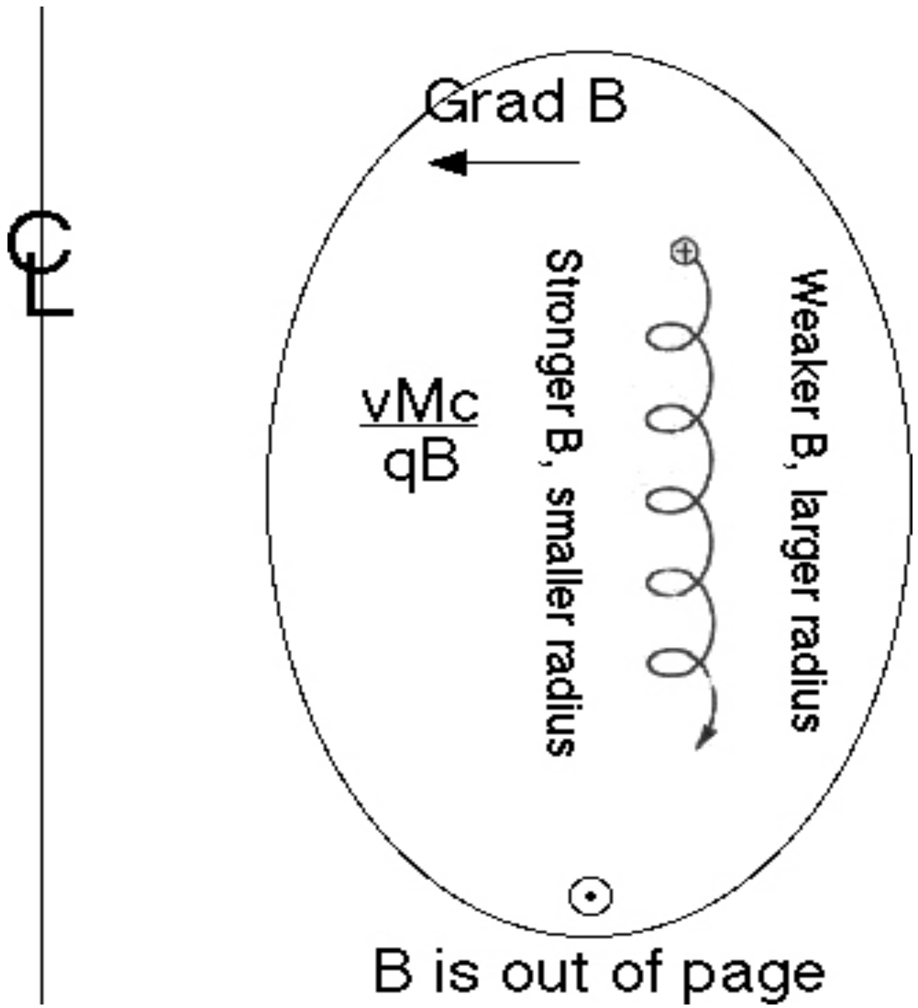
"But they will face many challenges, chief among them developing the ability to prevent instabilities in the edges of the plasma that can damage the experiment."

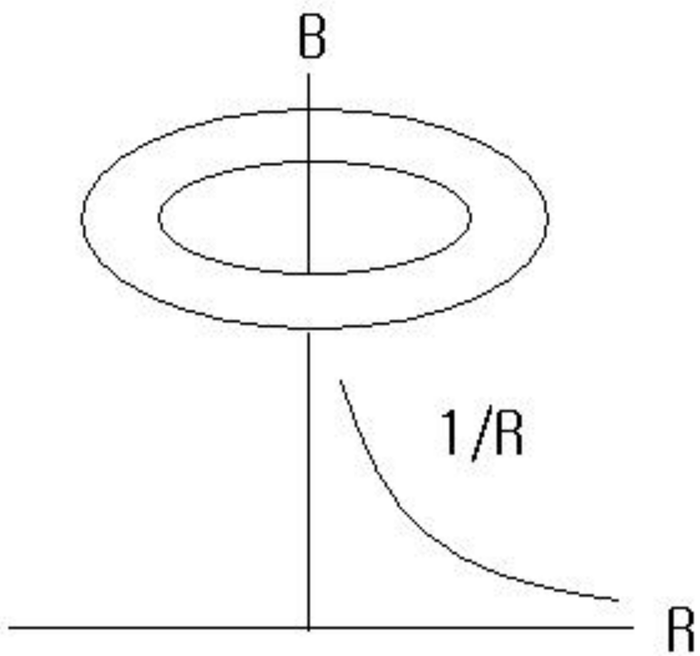


An advanced kinetic code has been constructed that can simulate the edge region in high fidelity → XGC

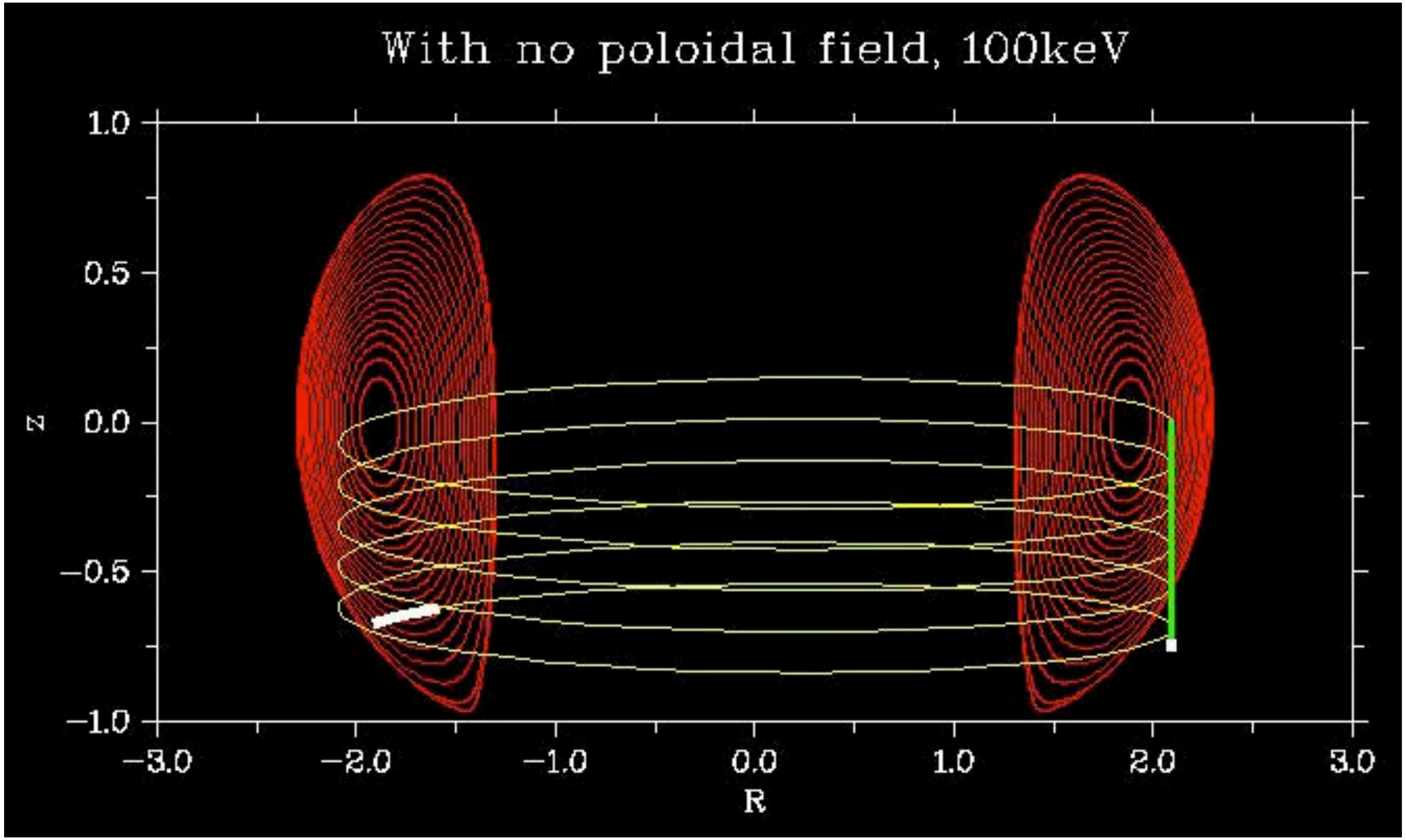
In a simple 2D toroidal B field without an adequate poloidal B field, particles are not confined even without any instabilities

Charged particles drift up or down.





Without poloidal magnetic field, particles are not confined

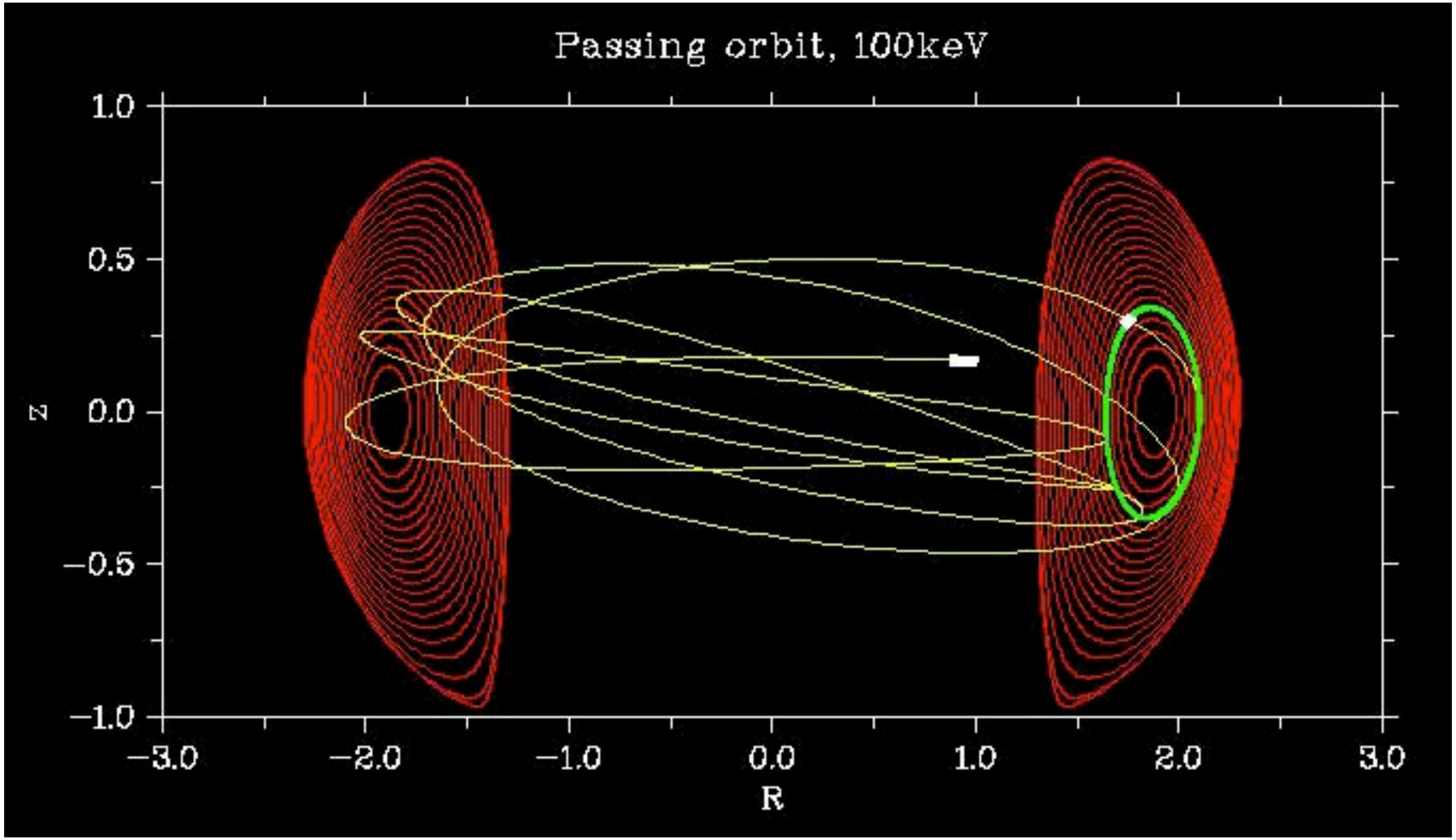


The flux surfaces shown here actually do not exist without poloidal magnetic field.

Gyromotions are not shown.

Visualization by
Sang-Hee Hahn

By adding B_{POL}, flux-surfaces are formed, vertical drift motion is cancelled between top & bottom, and single particle orbit is confined

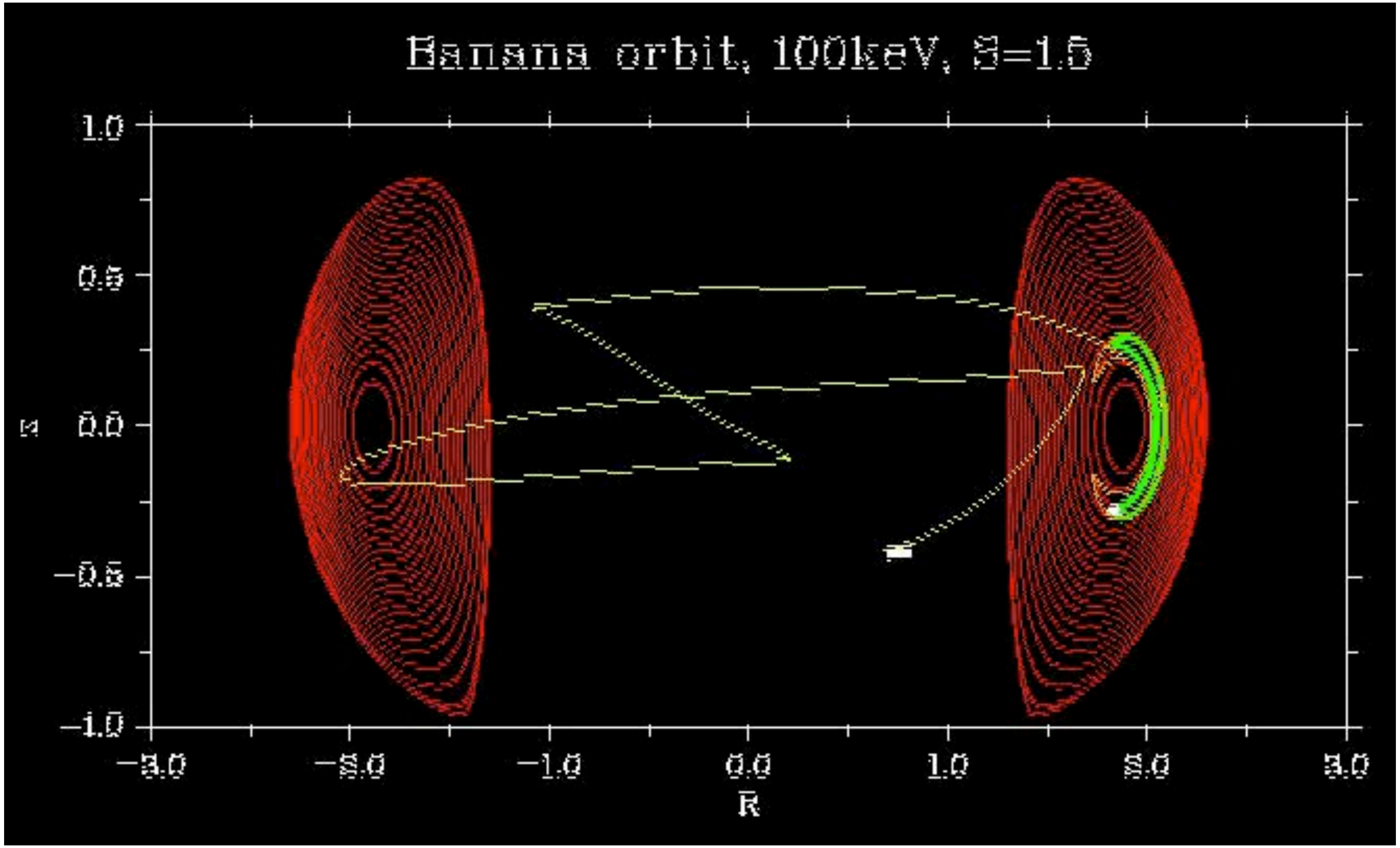


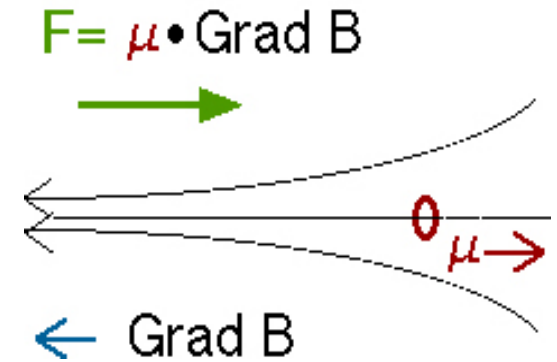
B_{POL} is added by either

- toroidal current (tokamak), or
- twisted external coils (stellarator)

Visualization by Sang-Hee Hahn

Magnetic mirror force creates trapped “banana” orbits





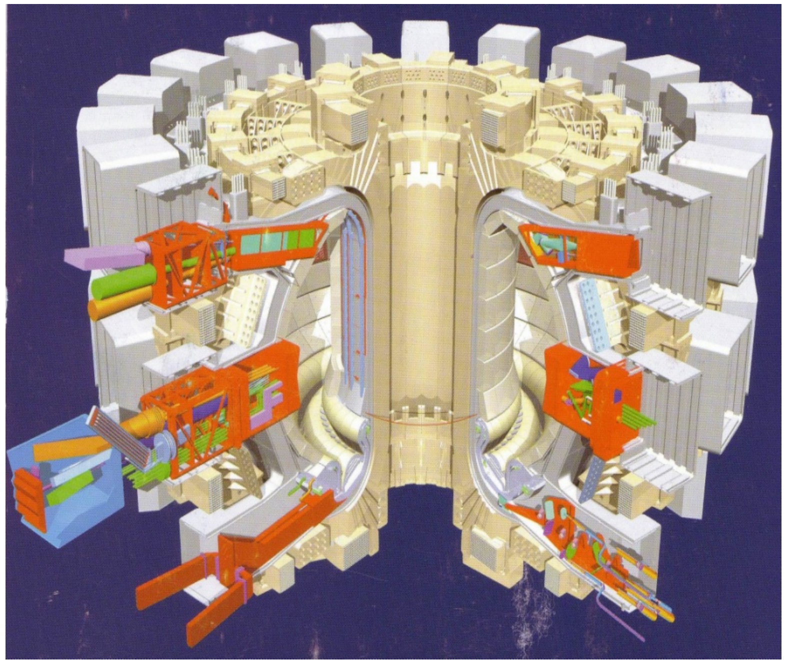
For “trapped” particles satisfying $\mu > \mu_C$

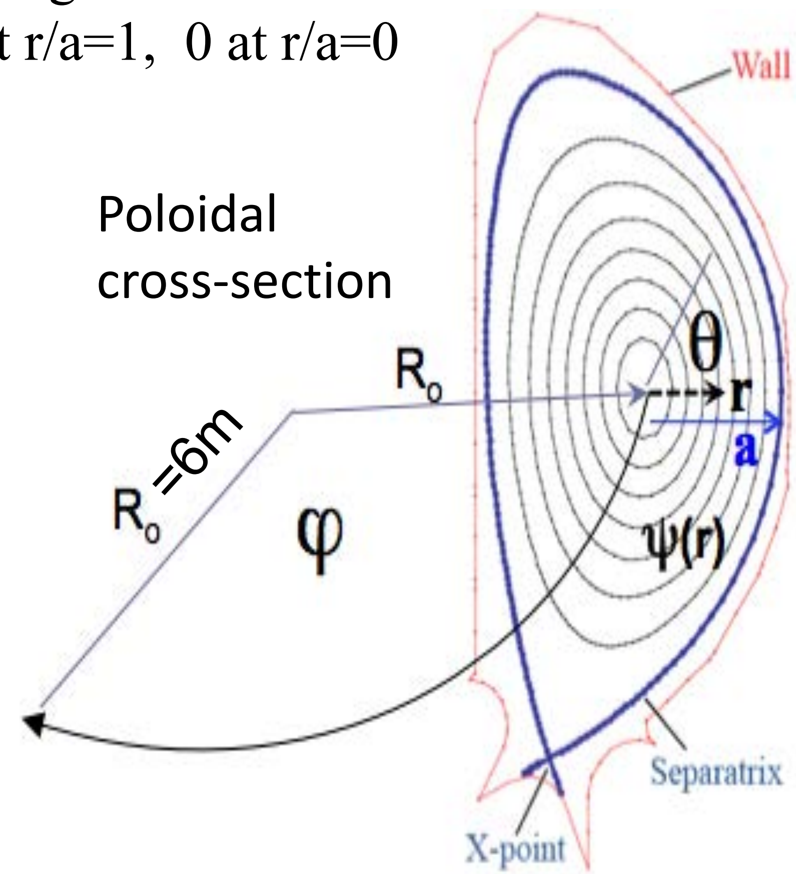
Yields “neoclassical” effects and begins to complicate the physics, with large collisional stepsize.

Visualization by Sang-Hee Hahn

Torus with twisted magnetic field complicates math & physics

Poloidal magnetic flux label
$\psi(r) = 1$ at $r/a=1$, 0 at $r/a=0$





Spatial inhomogeneity (neoclassical and ballooning effects, and **toroidal-poloidal mode coupling**.

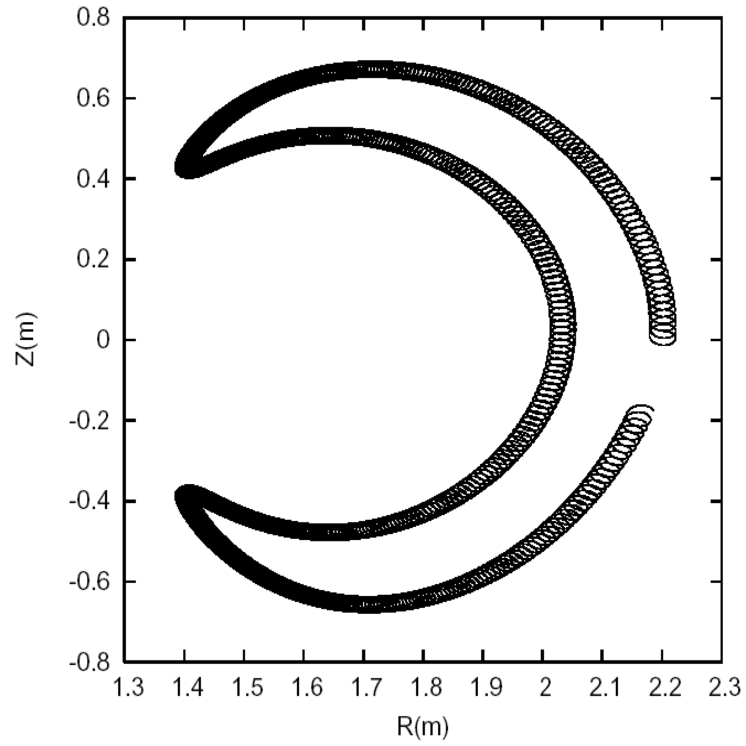
→ **≳10,000 particles per PIC cell**

→ **Requires trillion particles, minimally, to describe most important ITER physics**

→ **Extreme scale simulation → Exascale HPCs, minimally, will be needed complete physics.**

To enable kinetic simulation on today's HPCs, 6D Vlasov/ Fokker-Planck equations are reduced to 5D

- **Burning plasmas shall be free of the violent MHD-type instabilities**
  → Slow time-scale ($\omega << \Omega_I$) physics describes a burning fusion reactor plasma



Reduction of 6D to 5D by using a justifiable assumption:
"Gyro motion is much faster than the time scale of interest"

→Analytic treatment of the gyro-angle velocity variable α (gyro-averaging of the equations), while following the gyro-center motion

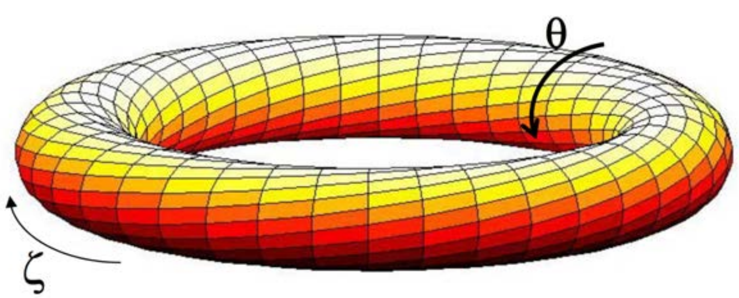
→Gyro-averaged Vlasov equation, while keeping the ab initio plasma physics intact: Landau resonance

→ Gyrokinetic Eqs. (3D in x and 2D in v), which do not use any empirical or ad hoc closures, hence are still first-principles equations within the justifiable assumption $\omega << \Omega_I$.

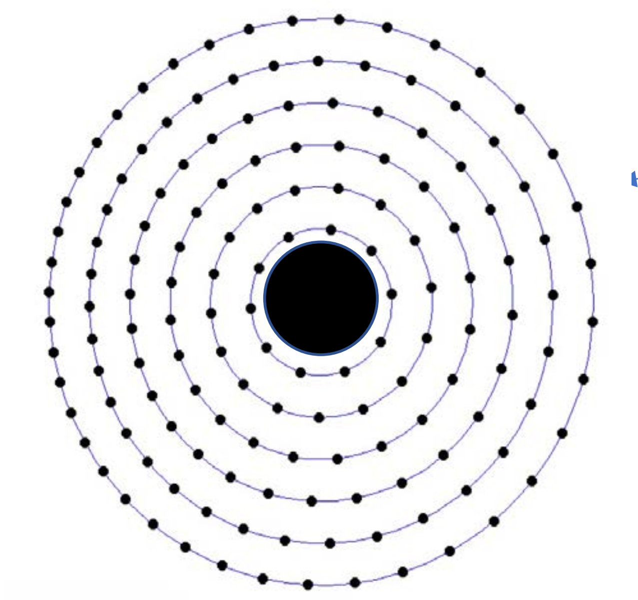
Two schemes to solve the 5D gyrokinetic equations for magnetic fusion physics

1. Total-f scheme: Solve the 5D gyrokinetic equation without further simplification
    - Necessary for edge plasma which is far from equilibrium
    - Contains all scale multi-physics without scale-separation as long as $\omega \ll \Omega_I$
    - Turbulence self-organizes with the large scale profile to self-organized-criticality (SOL)
    - Requires extreme scale computing
        - # particles per PIC cell ~10,000 → ~Trillions total particle for ITER
2. Delta-f scheme: Assume the plasma is well confined and in near equilibrium
    - $f=f_M + \delta f$ and $\delta f/ f_M \ll 1$
    - Delecate multiscale interaction between the large scale and small scale is ignored. Evolution of the global f_M profile is usually determined by a transport modeling and SOL is not persued.
    - Popular for the core plasma when the plasma profiles are known from experiments (error?)
    - Designed to save computing time by >100
    - # particles per PIC cell ~50 → ~tens millions total particle for ITER

B-field following mesh is highly advantageous for $k_\perp >> k_{||}$

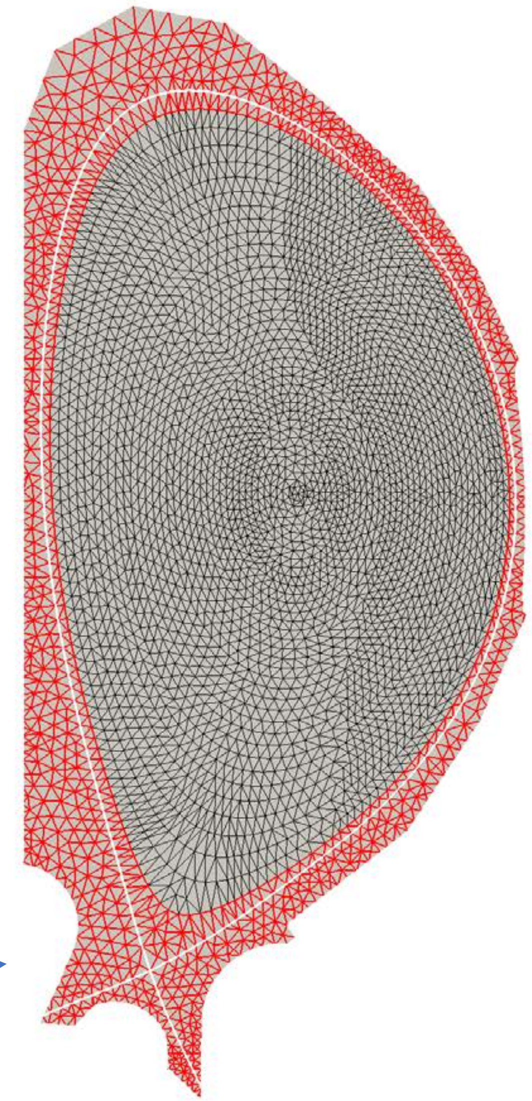


$$(\Psi, \alpha, \zeta) \Rightarrow \alpha = \theta - \zeta/q$$



GTC for core plasma

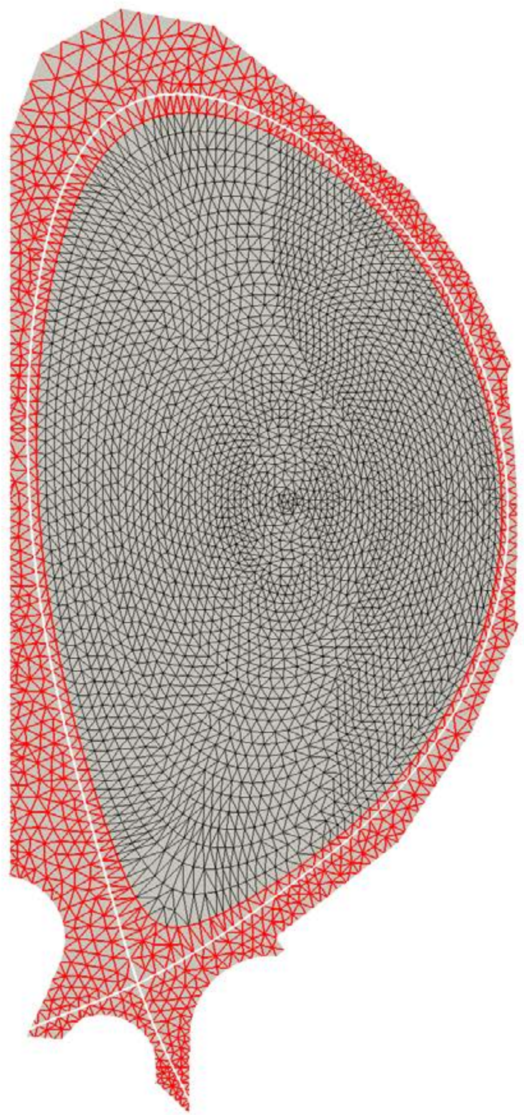
- In strong B, physics is highly stretched along the B-lines (flute)
  - B-field following mesh saves computing time by ~100x
- In the **core** plasma comfortably inside the magnetic surface, a magnetic coordinate system saves computing time, further.
  - Straight B-line
  - (Semi-)structured rectangular mesh is good enough
  - Mathematical singularity at separatrix, though
- For the core-**edge** whole-volume simulation, unstructured triangular mesh is logically advantageus
  - But, computationally expensive



XGC for edge-core

From now on, we will focus on the total-f scheme on leadership class HPCs

- Most of the core gyrokinetic codes in magnetic fusion plasma research utilize the delta-f scheme in magnetic coordinate system to enable smaller scale computing
  - To enable smaller scale computing
  - Not applicable to the general GEC problems
- GEC community may need to use the total-f/full-f scheme
  - Grid construction will be device-dependent
    - Unstructured, structured, block, triangular, AMR,…
    - Untructed triangular grid is highly flexbile in the geometric description, but adds complication (especially to particle sorting).
  - Non-Maxwellian collision operator should be used
    - We have a conservative Fokker-Planck-Landau scheme
  - First-principles GEC 6D simulation in realistic device geometry with many species and complicated atomic/molecular interaction may require leadership class computing



Fluid simulation with Fick's law type diffusive transport is not recommended for the far-from equilibrium plasma

For simplicity, let's use the drift kinetic equation for this argument

$$\frac{\partial f}{\partial t} + (v_{||} + v_d) \cdot \nabla f + \frac{e}{m} E_{||} v_{||} \frac{\partial f}{\partial w} = C(f,f) + \text{Sources/Sinks}$$

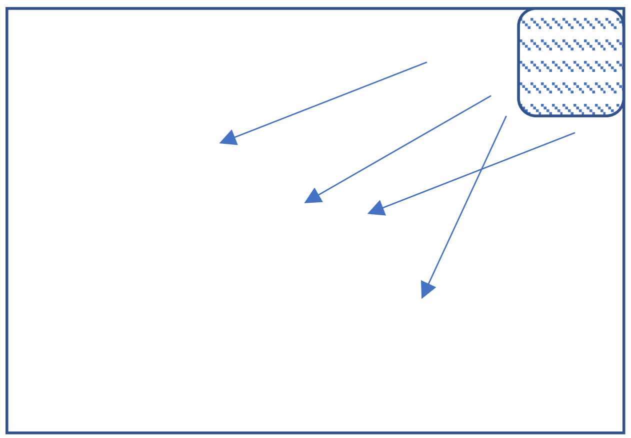
Plasma distribution function f evolves on the fast particle flight time

- Non-Maxwellian: $f \neq f_M$;

  $C(f)$, $v_{||}/L_{||}$, v_d/L_r, $ev_{||}E_{||}/T$, $S = O(\omega_{bi})$

- $\partial f/\partial t = O(\omega_{bi})$,
  - and find equilibrium from source and sink balance
- $\partial f/\partial t$ from a fluid simulation is on diffusive time scale
  - and much much slower.
  - Physics dynamics will also be inaccurate

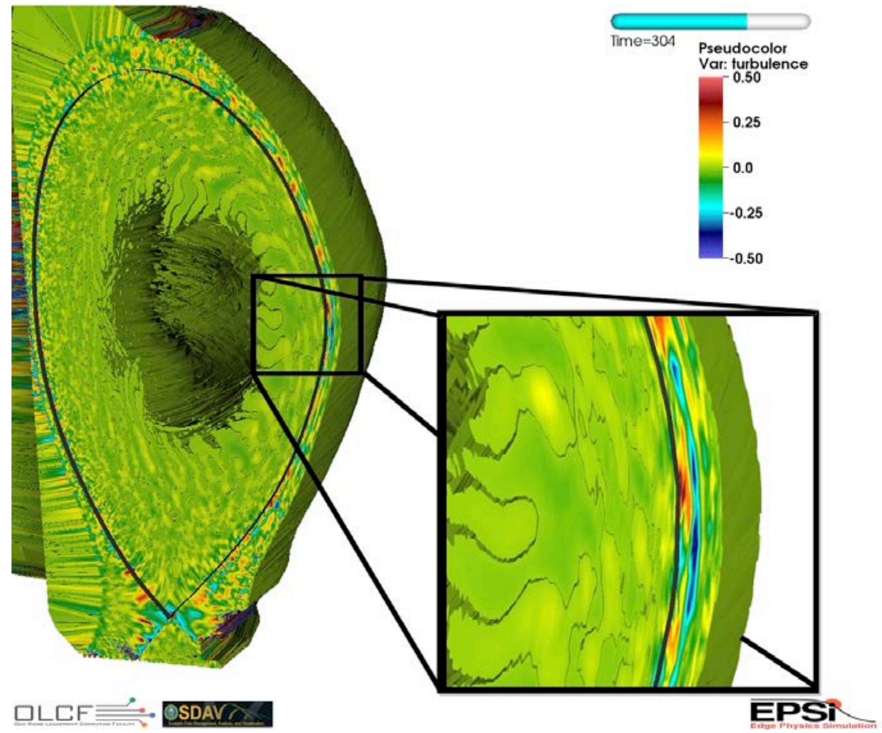
Particle equilibration in a box



XGC (X-point Gyrokinetic Code) is a unique gyrokinetic code in the world fusion program

- **Models the whole-volume, in contact with material wall and heat and momentum source in the core**
  - Study far-from-equilibrium plasma (non-Maxwellian)
  - Heat, momentum and particle sources are included
  - Monte-Carlo neutral particle recycling with atomic data
  - Fully nonlinear Fokker-Planck collision operation
- **Study overlapping multiscale, multi physics in space-time**
- **Big non-Mawellian physics per simulation time step**
  - ideal for big computers
- **Is a preferred code at leadership computing centers: selected into all three exascale programs with staff supports.**
- **Also, a DOE ECP (Exascale Computing Program) code**
- **>1 Billion core-hours of computing time awarded for 2019**

Boundary turbulence saturates in ≲0.1ms, while core turbulence does in a few ms.

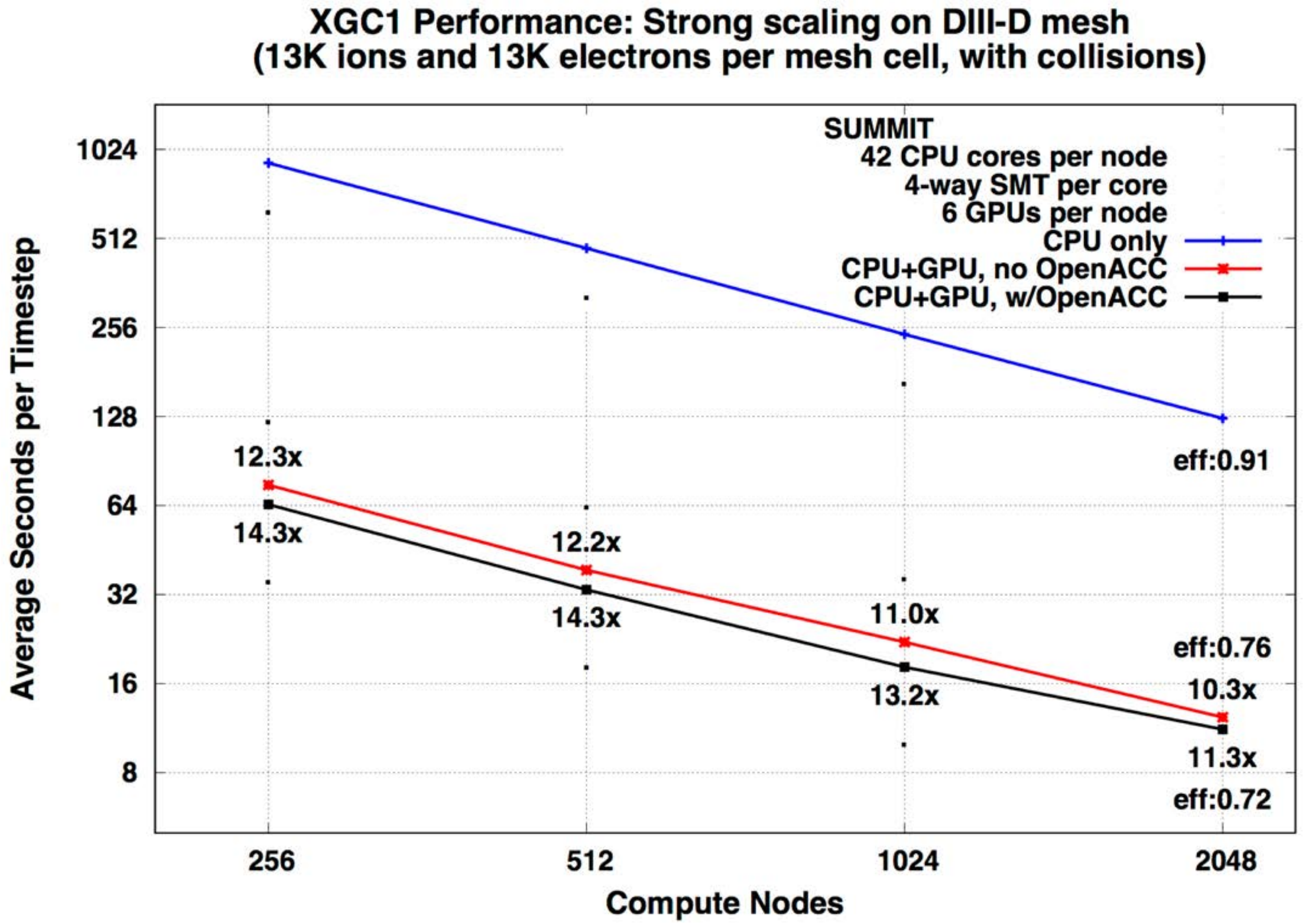


XGC Scales well on the new world #1 Summit

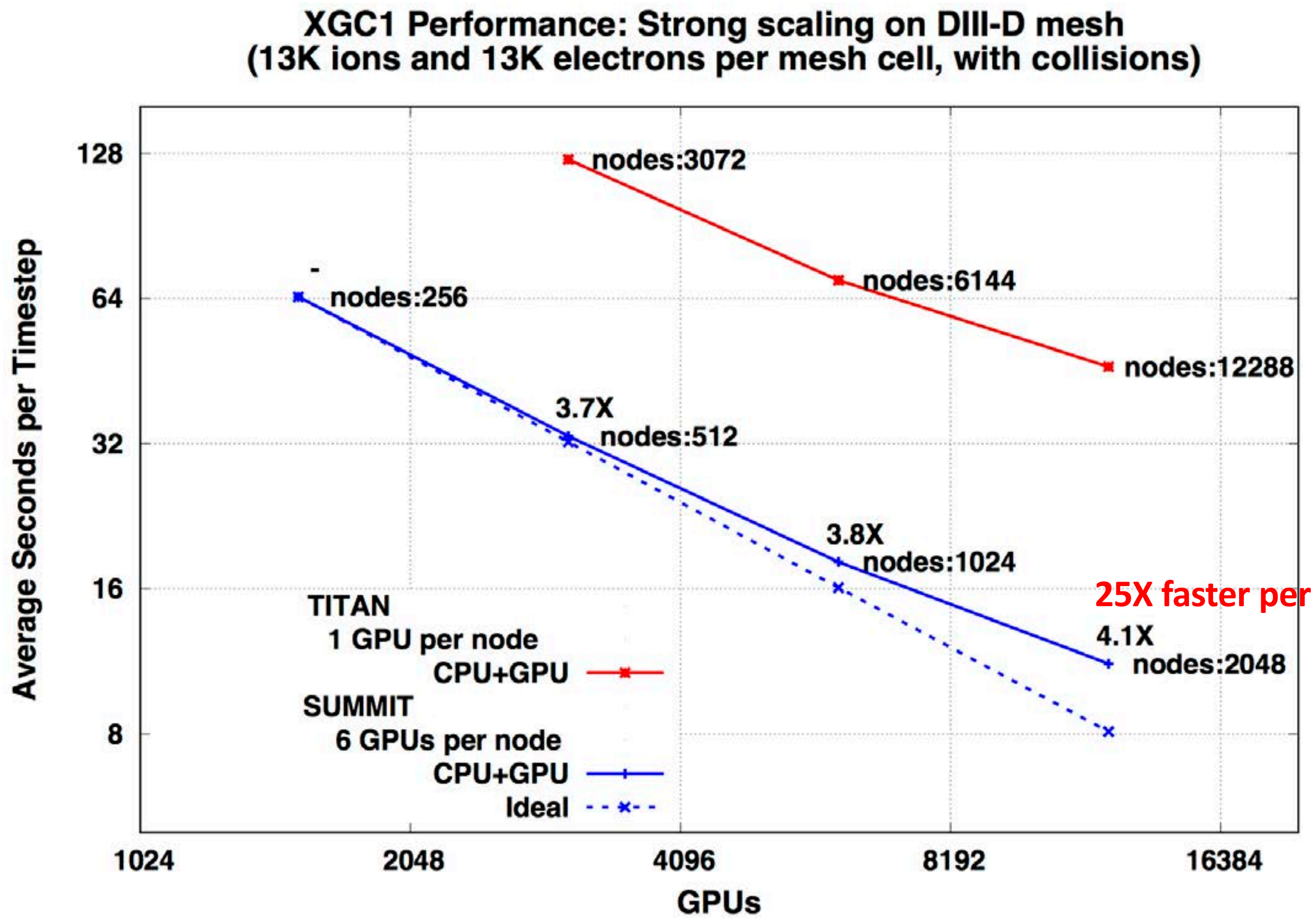
- XGC also scales well on the new world #1 Summit to the maximal available # nodes (2,048, near 50% capacity): one of first such codes.
- Using a **present production** case (underusing the GPU capability) on 2048 Summit nodes, XGC shows 11.3x speedup on GPU+CPU from CPU only.

Multi-level parallelization:

MPI + OpenMP + CUDA + OpenACC



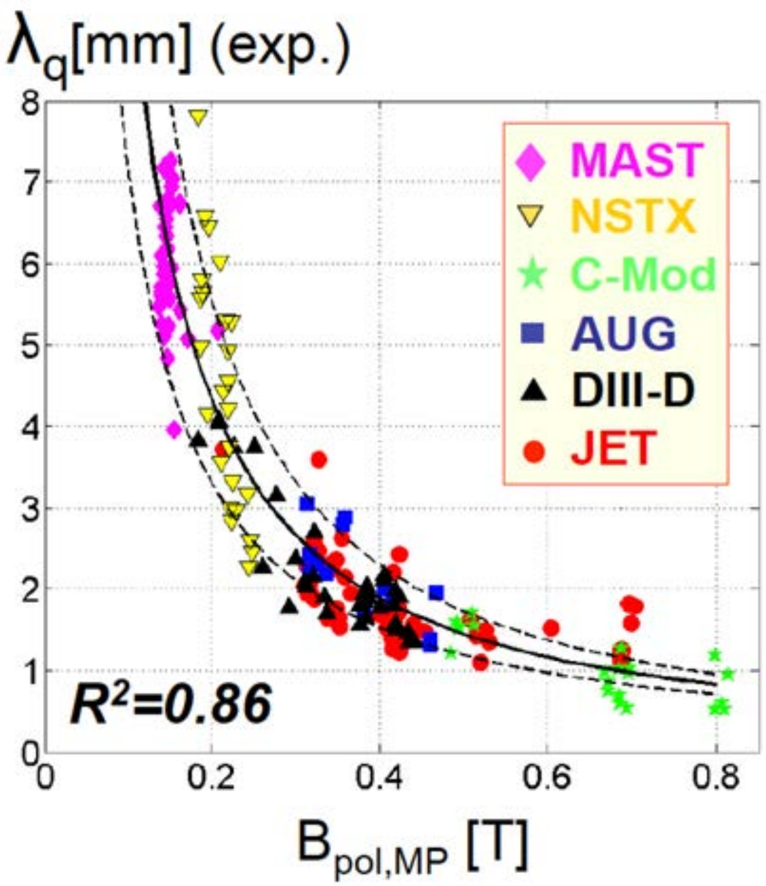
The production XGC is ≃25X faster per Summit node than per Titan node at 2,048 (44.4%) Summit nodes
(The theoretical ratio is 30)

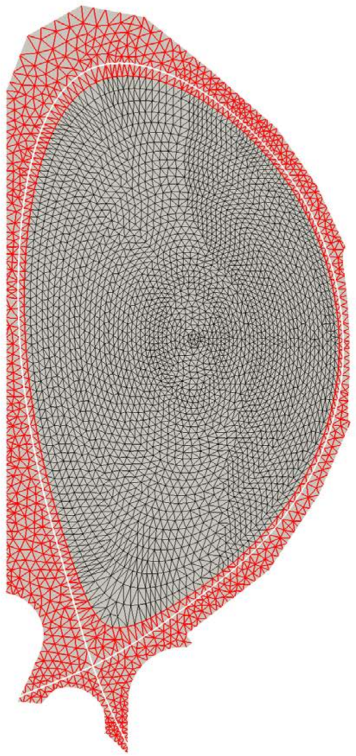


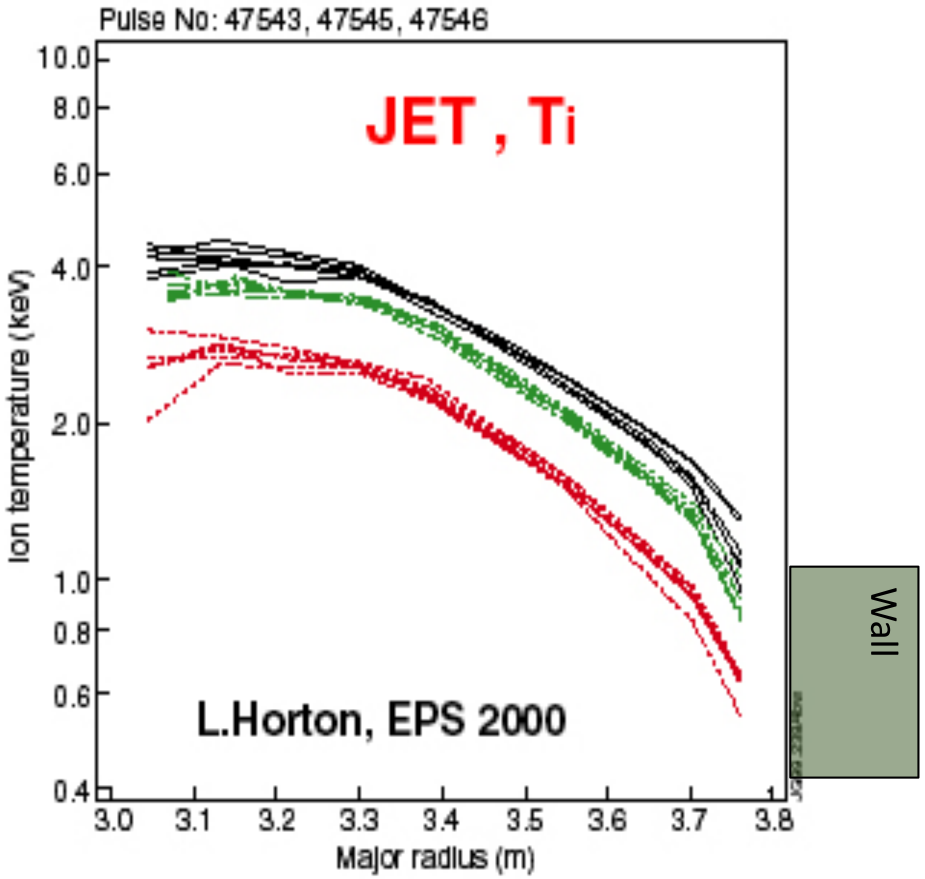
25X faster per node out of the theoretic factor 30.

Our early science study on Summit will start soon.

Understanding edge non-thermal physics is critical for ITER



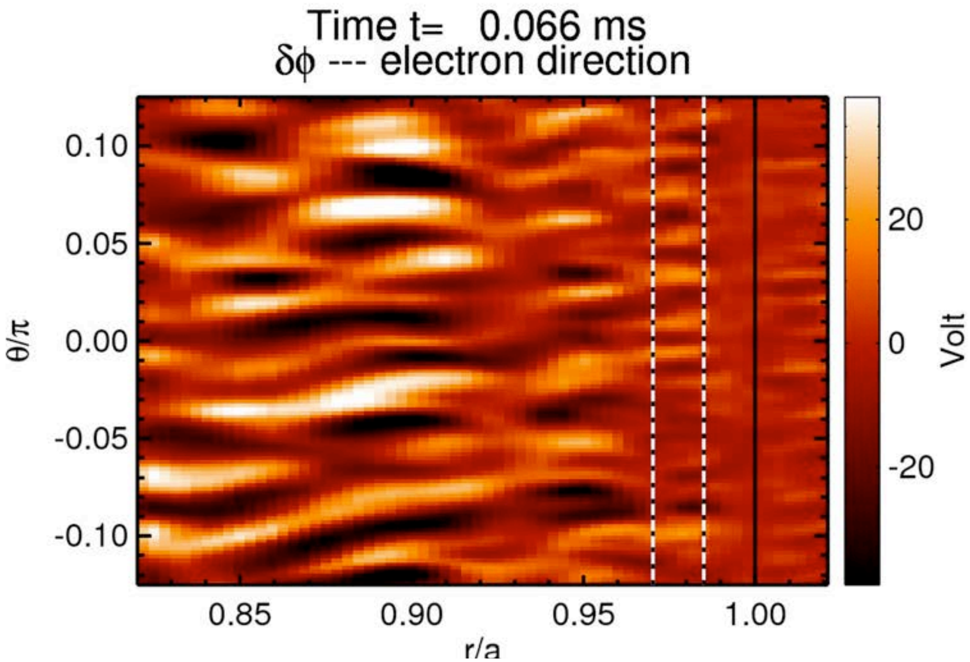


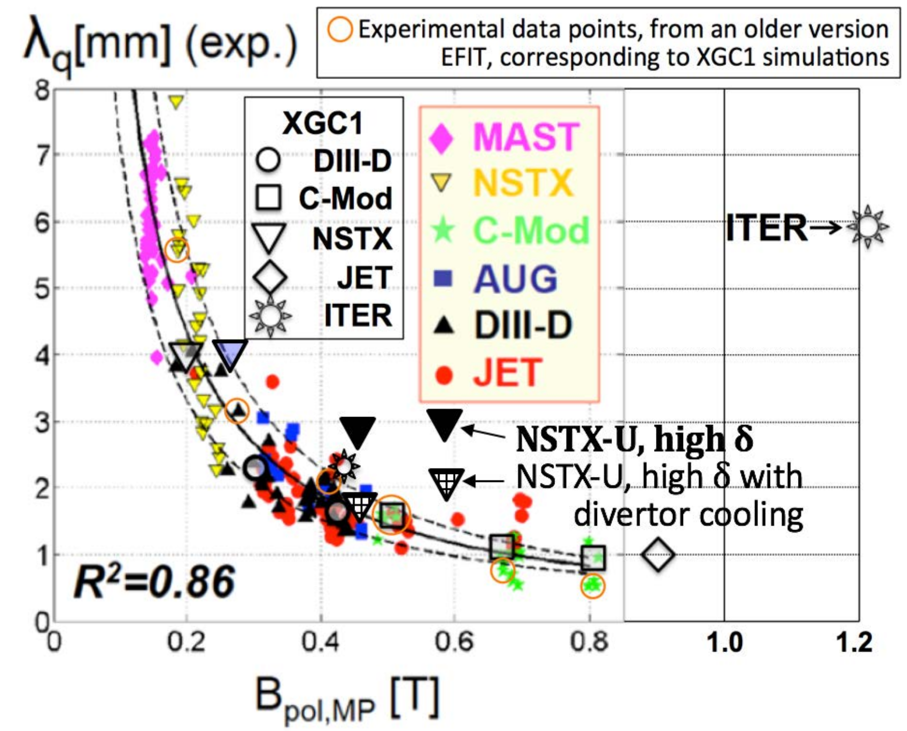


- Present tokamaks predicts that the heat-flux width on ITER will be too narrow for comfortable operation of ITER at full power.
- Will ITER obey the same physics?

- ITER relies on the achievement of the Low-to-High (L-H) confinement mode bifurcation
  - High edge pedestal → high core pressure
- How is the spontaneous L-H bifurcation occurring?

Finally, gyrokinetic findings of L-H bifurcation and divertor heat-flux width



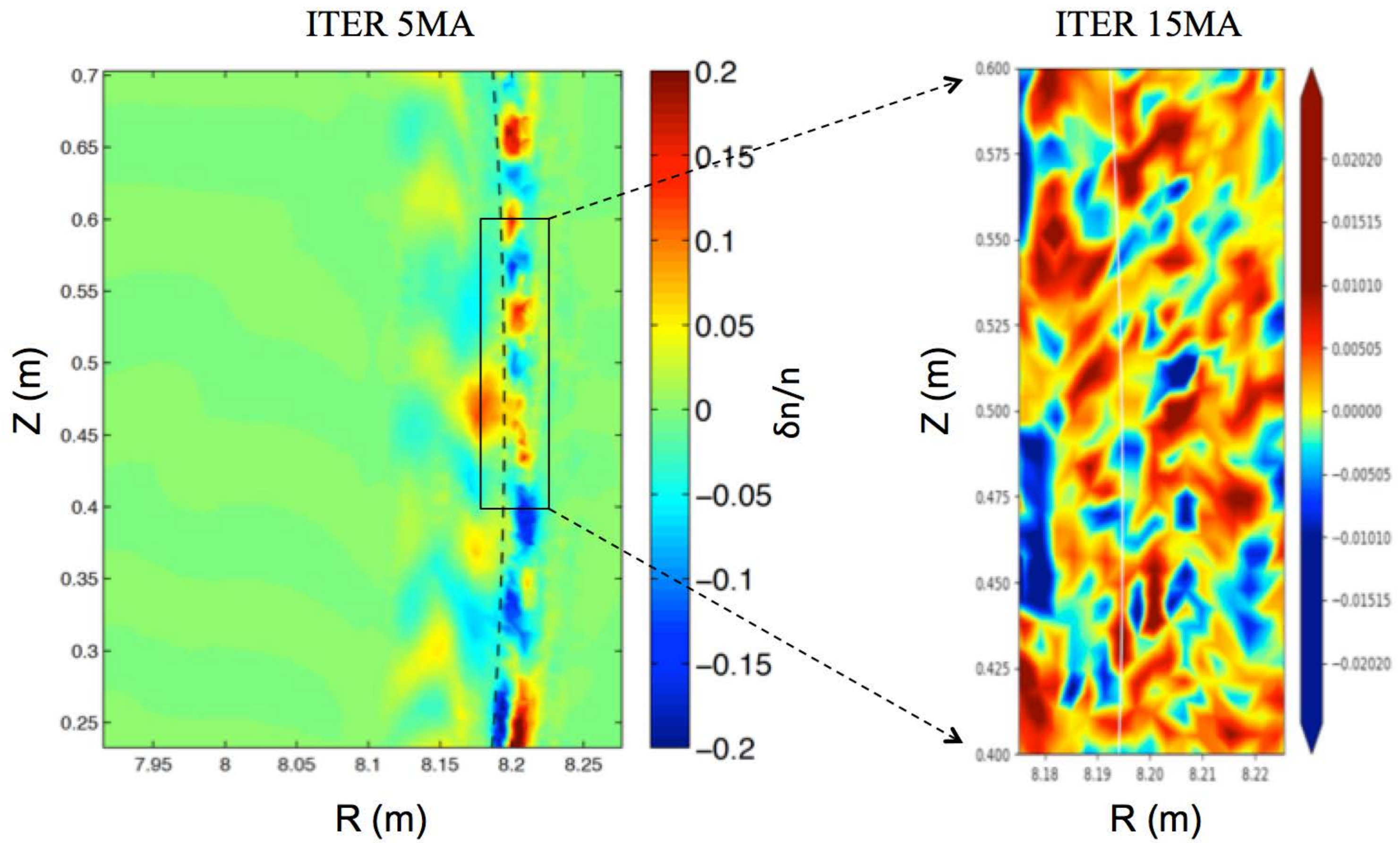


- ITER relies on the achievement L-H bifurcation
  - But, a kinetic understanding has been absent
- Gyrokinetic XGC finds that ExB shearing from turbulent Reynolds stress and neoclassical physics are not exclusive, but work together
- This understanding opens door to predicting the heating-power requirement for ITER.

[C.S. Chang, PRL 2017]

- ITER's divertor heat-load width is concern
  – Kinetic simulation is needed
- XGC agrees with existing tokamaks
- XGC on 15MA ITER shows flux width much wider than concern ~ design value
- Due to trapped electron turbulence, instead of blobby turbulence of today's tokamaks
  – Verified by studying NSTX-U

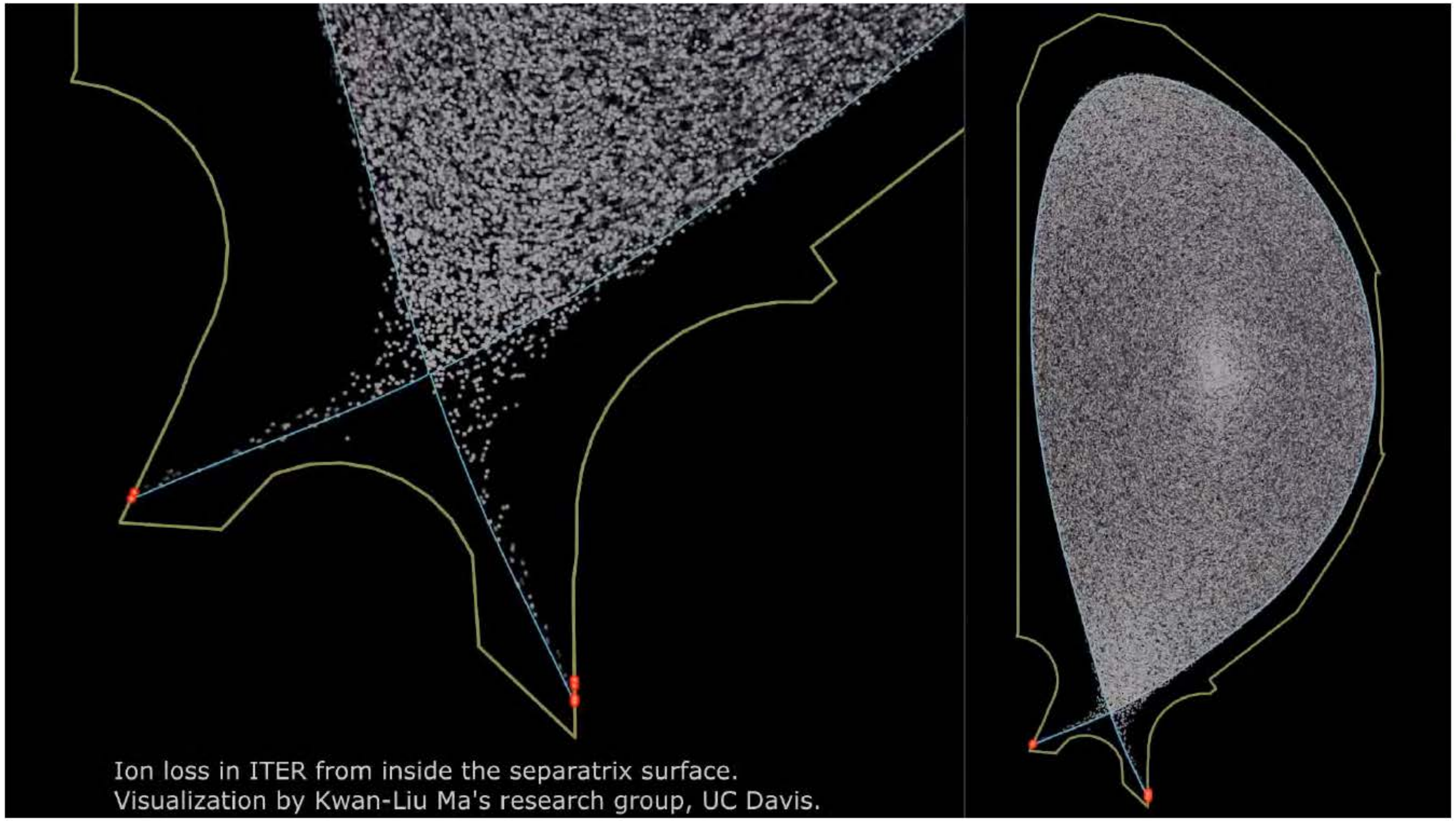
Evidence for an edge physics bifurcation between the higher and lower ρ_i/a values



Isolated "blobby" turbulence with strongly sheared ExB flow across separatrix

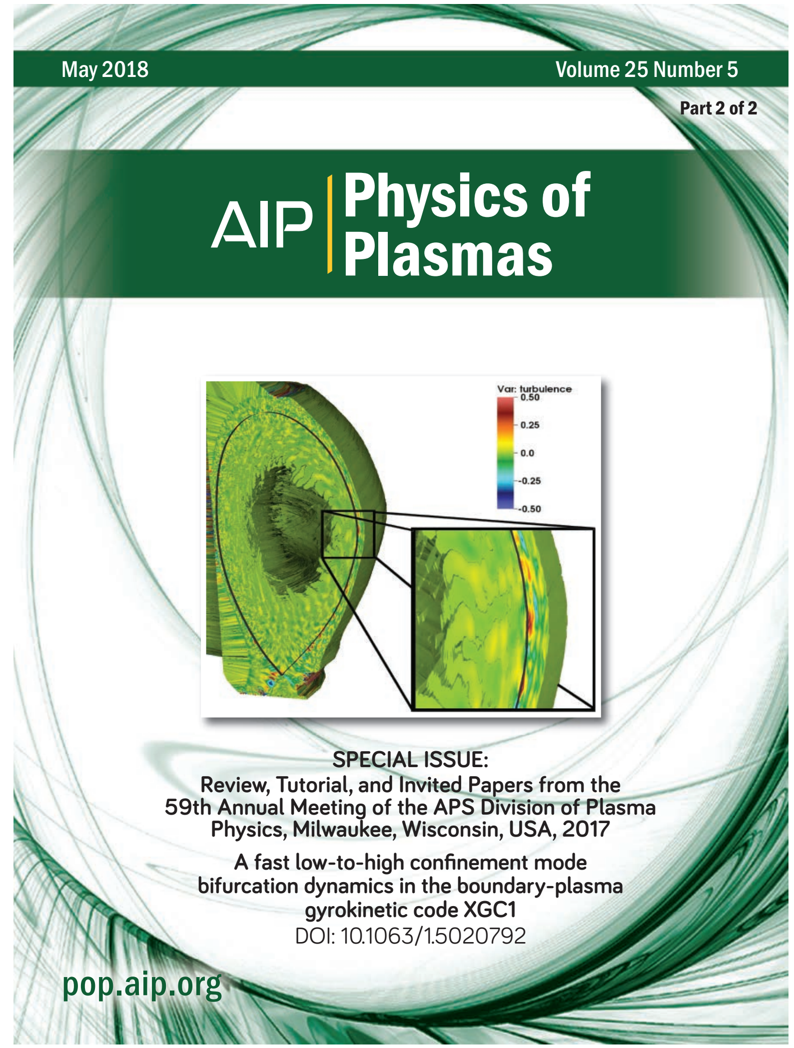
Connected, streamer-type trapped-electron turbulence with weakly sheared ExB flow

Particle simulation can reveal the high-fidelity physics at detailed level



ITER

Our Scientific Discoveries on Leadership Class HPCs have been featured at many places



But, there are many difficult hurdles to overcome for exascale computing in two different lanes.